

*trans*-Dichlorobis(3,4-lutidine- $\kappa$ N)palladium(II)

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## Key indicators

Single-crystal X-ray study

$T = 293$  K

Mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å

$R$  factor = 0.032

$wR$  factor = 0.084

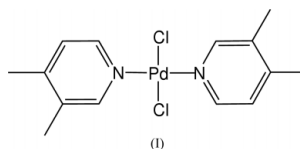
Data-to-parameter ratio = 21.0

For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.

In the title compound, *trans*-[PdCl<sub>2</sub>(C<sub>7</sub>H<sub>9</sub>N)<sub>2</sub>], the Pd atom lies on a crystallographic inversion centre and adopts a perfect square-planar coordination, with two chloride ligands at 2.2957 (6) Å and two N atoms of the 3,4-lutidine molecules at 2.0252 (17) Å from the Pd atom.

## Comment

The title compound, (I), was prepared in the course of our studies as a precursor to other palladium compounds. The easy access to suitable single crystals allowed us to carry out an X-ray diffraction study.



The Pd atom lies on an inversion centre and the ligands are therefore arranged in a *trans*-geometry. The Cl—Pd—N angles are 89.95 (6) and 90.05 (6)°, and the Cl—Pd—Cl<sup>i</sup> and N—Pd—N<sup>i</sup> angles are precisely 180° [symmetry code: (i)  $-x, -y, -z$ ]. These structural parameters imply a perfect square-planar geometry around the Pd<sup>II</sup> centre. The Pd—Cl and Pd—N distances are 2.2957 (6) and 2.0252 (17) Å, respectively. These bond lengths are comparable to those observed in *trans*-[PdCl<sub>2</sub>(pyridine)<sub>2</sub>], (II) (Viostat *et al.*, 1993), *trans*-[PdCl<sub>2</sub>(2,6-lutidine)<sub>2</sub>], (III) (Losier *et al.*, 1996), and *trans*-[PdCl<sub>2</sub>(2-Et-pyridine)<sub>2</sub>], (IV) (Biagini *et al.*, 1999). In (I), the Pd/N/Cl plane makes an angle of 55.2 (1)° with the plane formed by the 3,4-lutidine ligands, in contrast to the situations in (III) and (IV), where the aromatic rings are nearly orthogonal to the coordination plane.

## Experimental

The title compound was isolated as a by-product of the reaction of the dimeric complex  $[(\eta^3\text{-Ind})\text{Pd}(\mu\text{-Cl})_2]$  (Ind is indene) (200 mg, 0.39 mmol) with 3,4-lutidine (88  $\mu$ l, 0.78 mmol) in diethyl ether (20 ml) at room temperature. After stirring for 45 min, a yellow powder precipitated and was isolated by filtration. Recrystallization of a small portion of this solid from a CH<sub>2</sub>Cl<sub>2</sub> solution yielded crystals suitable for X-ray diffraction study.

## Crystal data

[PdCl<sub>2</sub>(C<sub>7</sub>H<sub>9</sub>N)<sub>2</sub>]  
 $M_r = 391.60$   
Monoclinic,  $P2_1/n$   
 $a = 8.2331$  (9) Å  
 $b = 7.0910$  (5) Å  
 $c = 13.5417$  (13) Å  
 $\beta = 99.338$  (8)°  
 $V = 780.10$  (13) Å<sup>3</sup>  
 $Z = 2$

$D_x = 1.667$  Mg m<sup>-3</sup>  
Mo  $K\alpha$  radiation  
Cell parameters from 25  
reflections  
 $\theta = 15.0\text{--}30.0^\circ$   
 $\mu = 1.52$  mm<sup>-1</sup>  
 $T = 293$  (2) K  
Block, orange–yellow  
 $0.60 \times 0.54 \times 0.30$  mm

Data collection

Siemens P4 diffractometer  
 $\theta$ -2 $\theta$  scans  
 Absorption correction:  $\psi$  scan  
 (North *et al.*, 1968)  
 $T_{\min} = 0.415$ ,  $T_{\max} = 0.630$   
 7236 measured reflections  
 1886 independent reflections  
 1755 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.039$   
 $\theta_{\text{max}} = 28.0^\circ$   
 $h = -10 \rightarrow 10$   
 $k = -9 \rightarrow 9$   
 $l = -17 \rightarrow 17$   
 3 standard reflections  
 every 97 reflections  
 intensity decay: none

Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.032$   
 $wR(F^2) = 0.084$   
 $S = 1.18$   
 1886 reflections  
 90 parameters  
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0481P)^2 + 0.2651P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} < 0.001$   
 $\Delta\rho_{\text{max}} = 0.39 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\text{min}} = -1.74 \text{ e } \text{\AA}^{-3}$

Table 1

Selected geometric parameters ( $\text{\AA}$ ,  $^\circ$ ).

Pd—N	2.0252 (17)	C2—C3	1.404 (3)
Pd—Cl	2.2957 (6)	C2—C6	1.498 (3)
N—C1	1.342 (3)	C3—C4	1.375 (3)
N—C5	1.346 (3)	C3—C7	1.504 (3)
C1—C2	1.384 (3)	C4—C5	1.384 (4)
$N^i$ —Pd—N	180	C1—C2—C3	118.2 (2)
N—Pd—Cl	89.95 (6)	C1—C2—C6	119.9 (2)
N—Pd—Cl <sup>i</sup>	90.05 (6)	C3—C2—C6	121.9 (2)
Cl—Pd—Cl <sup>i</sup>	180	C4—C3—C2	118.1 (2)
C1—N—C5	118.31 (19)	C4—C3—C7	120.5 (2)
C1—N—Pd	121.93 (14)	C2—C3—C7	121.4 (2)
C5—N—Pd	119.76 (16)	C3—C4—C5	120.6 (2)
N—C1—C2	123.3 (2)	N—C5—C4	121.5 (2)

Symmetry code: (i)  $-x, -y, -z$ .

All H atoms were placed in calculated positions, with C—H distances of 0.93 (phenyl) and 0.96  $\text{\AA}$  (methyl), and were included in the refinement in riding-model approximation, with  $U_{\text{iso}} = 1.5U_{\text{eq}}$  for methyl H atoms and  $1.2U_{\text{eq}}$  for all others. In the final difference Fourier map, the first peak ( $0.39 \text{ e } \text{\AA}^{-3}$ ) were located  $0.87 \text{ \AA}$  from the Pd atom and the the general background was found to be less than  $0.37 \text{ e } \text{\AA}^{-3}$ .

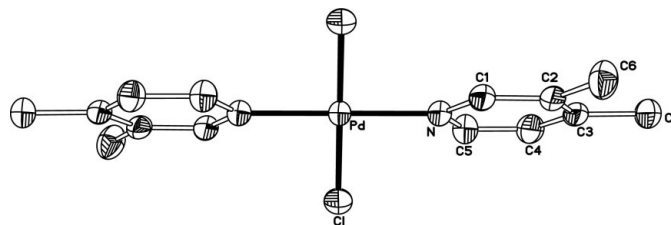


Figure 1

View of the title molecule. Displacements ellipsoids are drawn at the 50% probability level and H atoms have been omitted. The unlabelled part of the molecule is related by the symmetry code  $(-x, -y, -z)$ .

Data collection: XSCANS (Siemens, 1995); cell refinement: XSCANS; data reduction: XSCANS; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Bruker, 1997); software used to prepare material for publication: UDMX (local program).

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